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09/506,717	02/18/2000	Harold E Helson	103544.127	9161

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EXAMINER

DEJONG, ERIC S

ART UNIT	PAPER NUMBER
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1631

DATE MAILED: 06/13/2005

Please find below and/or attached an Office communication concerning this application or proceeding.

Office Action Summary

Application No.

09/506,717

Applicant(s)

HELSON, HAROLD E

Examiner

Eric S. DeJong

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-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --
Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If the period for reply specified above is less than thirty (30) days, a reply within the statutory minimum of thirty (30) days will be considered timely.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

Status

- 1) ☒ Responsive to communication(s) filed on 22 April 2005 and 28 October 2004.
- 2a) ☐ This action is FINAL. 2b) ☒ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

Disposition of Claims

- 4) ☒ Claim(s) 5-16 and 19-21 is/are pending in the application.
- 4a) Of the above claim(s) _____ is/are withdrawn from consideration.
- 5) ☐ Claim(s) _____ is/are allowed.
- 6) ☒ Claim(s) 5-16 and 19-21 is/are rejected.
- 7) ☐ Claim(s) _____ is/are objected to.
- 8) ☐ Claim(s) _____ are subject to restriction and/or election requirement.

Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☐ The drawing(s) filed on _____ is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All b) ☐ Some * c) ☐ None of:
- ☐ Certified copies of the priority documents have been received.
 - ☐ Certified copies of the priority documents have been received in Application No. _____.
 - ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

* See the attached detailed Office action for a list of the certified copies not received.

Attachment(s)

- ☒ Notice of References Cited (PTO-892)
- ☐ Notice of Draftsperson's Patent Drawing Review (PTO-948)
- ☐ Information Disclosure Statement(s) (PTO-1449 or PTO/SB/08)
Paper No(s)/Mail Date _____
- ☐ Interview Summary (PTO-413)
Paper No(s)/Mail Date. _____
- ☐ Notice of Informal Patent Application (PTO-152)
- ☐ Other: _____

S. O. O.

DETAILED ACTION

ACKNOWLEDGEMENTS

Applicants arguments, filed on 04/22/2005 and 10/28/2004, have been fully considered but they are not deemed persuasive. They constitute the complete set presently being applied to the instant application. The amended set of claims, filed on 04/22/2005, replace all previous versions of the claims. Claims 1-4, 17, and 18 have been canceled. Claims 5-16 and 19-21 are currently under examination.

NEW MATTER

Applicants arguments and amendments made to instant claims 11, 13, 14, and 16 are found convincing and, therefore, the previous rejections claims 11, 13, 14, and 16 as containing NEW MATTER are withdrawn.

VAGUENESS AND INDEFINITENESS

Applicants arguments and amendments made to instant claims 10 and 16 are found convincing and, therefore, the previous rejections of claims 10 and 16 on the grounds of USC § 112, second paragraph, are withdrawn.

NON-STAUTORY SUBJECT MATTER

Applicants arguments and amendments to claims 5, 9, 10, 12, 20, and 21 to recite "outputting the fixed bond information" are found convincing and, therefore, the previous rejections of claims 5-16 and 19-21 under USC §101 are withdrawn.

SUBSTANTIAL CLAIM DUPLICATION

Applicant is advised that should claims 7 and 8 be found allowable, claims 7 and 8 will be objected to under 37 CFR 1.75 as being a substantial duplicate thereof. When two claims in an application are duplicates or else are so close in content that they both cover the same thing, despite a slight difference in wording, it is proper after allowing one claim to object to the other as being a substantial duplicate of the allowed claim. See MPEP § 706.03(k).

Claim Rejections - 35 USC § 102(a)

The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

A person shall be entitled to a patent unless –

(a) the invention was known or used by others in this country, or patented or described in a printed publication in this or a foreign country, before the invention thereof by the applicant for a patent.

Claims 5-16 and 19-21 are rejected under 35 U.S.C. 102(a) as being clearly anticipated by Glendening et al. This rejection is newly applied.

The pending claims are generally drawn to methods and systems for use in deriving fixed bond information from a delocalized structure representation. The claimed

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invention comprises the steps of analyzing a delocalized representation of a chemical structure that contains at least in part a polycyclic ring system, identifying a plurality of fixed bond representations candidates based on valence information, evaluating a subset of the fixed bond representations, selecting fixed bond representation candidates based on the evaluation, producing fixed bond information based on the selection and outputting said fixed bond information.

[Claims 5, 19, 20, and 21]: Glendening et al. sets forth a quantum-mechanical resonance theory based on a first-order reduced density matrix and a representation of chemical structures in terms of natural bond orbitals. A "natural" resonance theory is disclosed that leads to an optimal resonance-weighted approximation to the full density matrix, wherein the "single reference" limit of weak delocalization is combined with full "multireference" limit of strong delocalization. The results provide an intrinsic criterion of accuracy of the resonance-theoretic description. See Glendening et al., Abstract.

Glendening et al. sets forward an analysis program that takes as input a resonance structure and performs a quasi-quantum mechanical analysis on delocalized structures to establish natural bond orders (NBO) for formalized Lewis structures which read on the limitation of producing and outputting fixed bond information in a selected fixed bond structure. See Glendening et al., page 597, column 1, lines 15-39. The conceptual methodology employed in the algorithm rely on valence theory in establishing resultant fixed bond structure. See Glendening et al., page 597, lines 34-39. The disclosed methodology and system provides for the generation of several possible structures from a starting resonance or delocalized chemical input structure

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and a selection routine to pick from the generated structures the most plausible fixed structure candidate. See Glendening et al., page 602, column 2, line 13 through, page 604, column 1, line 29. The program is fully capable of accepting polycyclic structures as demonstrated on page 603, column 2, line 34 through page 604, column 1, line 3.

[Claim 6]: The disclosed methodology explicitly accounts for molecular situations where delocalization effects are so strong that no NBO Lewis structure is dominant. This is broadly construed as reading on a delocalized chemical representation with a hetero-substitution pattern. See Glendening et al., page 600, column 1, line 6 through column 2, line 8.

[Claims 7 and 8]: Specific examples are provided wherein the methodology is capable of accepting and operating on portions of delocalized chemical representation that describe a non-cyclic/acyclic system. See for example Glendening et al., page 594, column 1, line 17 through column 2, line 12. For the purposes of examination, the limitations of a non-cyclic system and acyclic system are both construed as chemical systems that do consist of a cyclical chemical structure.

[Claims 9 and 10]: The methodology set forth by Glendening et al. also accounts for producing fixed bond structures that include a pair of opposite charges as well as a pair of radicals that are lacked by the delocalized representation. See for example Glendening et al., page 597, column 2, lines 1-27.

[Claims 11 and 15]: The instant specification on page 6, lines 10-13, is relied upon for possible definition of an ESVD as the collection of characteristics pertaining to an atomic environment such as charge, any unpaired electrons, and bonding

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information. As such, Glendening et al. a delocalization list of NBO interactions of a parent reference structure used to generate a list of the associated secondary structures describing a delocalized hybrid. Given the formal resonance structures, the NBO program is able to calculate the optimal set of NBOs for a given structure. Under a reasonably broad interpretation these teaching read on the claimed limitation of identifying based on an ESVD as well as queing at least a subset of the ESVDs by priority.

[12-14]: Glendening et al. sets forth the use of the NRT program for sampling a wide vairiety of candidate structures. Said structures can be generated from several alternatives such as the Wiberg bond index, the delocalization lists for any previous list of candidate structures, or specified by the user of the program. See Glendening et al., page 598, column 1, line 38 through column 2, line 7. As such, under a reasonably broad interpretation, the disclosed methodology and systems read on the claimed limitation of using a pre-computed table. The alternatives presented by Glendening et al. also cover allowing additional elements and values to be added to the table as well as additions being applied to any chemical element.

[Claim 16]: The disclosed practicality of the NRT method is indicated by the computation time used to arrive at a particular or given set of structures. The methods and systems set forth in Glendening et al. are customizable so that either a set number of iterations are performed, thus providing a selectable longer or shorter set of expanded structures generated by the program. See Glendening et al., page 608, column 1, lines 1-36.

Claim Rejections - 35 USC § 102(b)

The following is a quotation of the appropriate paragraphs of 35 U.S.C. 102 that form the basis for the rejections under this section made in this Office action:

A person shall be entitled to a patent unless –

(b) the invention was patented or described in a printed publication in this or a foreign country or in public use or on sale in this country, more than one year prior to the date of application for patent in the United States.

Claims 5, 11, 15, and 20 are rejected under 35 U.S.C. 102(b) as being clearly anticipated by Graovac et al. This rejection is reiterated and maintained from the previous Office action, and as necessitated by amendments to the instant claims.

In regards to claim 5, applicant argues that Graovac et al. does not derive fixed bond representations from delocalized ones and is not concerned with deriving fixed bond information. Applicant assert that numerous definitions and references to delocalized structure representations are provided for on pages 23 through 24 and Figure 21 of the instant disclosure. Further, applicants assert that the method disclosed by Graovac et al. is only applicable to all-carbon systems. Applicants also assert that there is no disclosure or suggestion in Graovac et al. for the steps of analyzing a delocalized representation of a chemical structure, identifying based on valence information a plurality of fixed bond representation candidates, evaluating at least a subset of the fixed bond representation candidates, selecting candidates based on the evaluations, producing fixed bond information, and outputting the fixed bond information.

Applicants arguments and citations have been fully considered but are not found convincing. Consideration of pages 23 and 24 from the instant specification revealed

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specific implementations and examples of the disclosed methodology rather than an explicit definition of what is meant by the limitation of "delocalized structure representation". As such, the examiner reiterates that no instantly disclosed definition of what is meant by "delocalized structure representation" as in the instant claims has been found to distinguish over the representations shown in Figures 1 and 2 of Graovac et al. These figures are pointed to regarding delocalized structures as now presented in the instant claims. Such delocalized structures are reasonably interpreted to include chemical structures without localized fixed (conventional) bonds. Such non-fixed bond representations are shown in Figures 1 and 2 and analyzed and evaluated (instant claim 5, line 6, for example) regarding Kekule index contributions for the calculation of structures as numerous depicted throughout the reference. The assertion regarding applicability of the reference to all-carbon systems is also non-persuasive because instant claim 5 is directed to a polycyclic ring system and is not limited so as to exclude all-carbon systems thus including the systems of Graovac et al. Applicant argues that there is no suggestion of outputting the fixed bond information in Graovac et al., however Table I clearly displays a resultant set of arranged polycyclic ring structures with fixed bond information.

In regards to claims 11 and 15, applicant further argues that there is no disclosure in Graovac et al. for priority queuing as set forth in the present claims. Applicant acknowledges that Table I of Graovac et al. illustrates certain values have been selected as input for calculating the Kekulé index for individual valence structures of several polycyclic systems and that this compilation is sorted in a desired order.

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No instantly disclosed definition of what is means by "queuing... by priority " as in the instant claims has been found to distinguish over the representations shown in Table I of Graovac et al. Contrary to applicants assertion, it is therefore reasonably concluded that a the described compilation sorted in a desired order reads on the claimed limitation of queuing at least a subset of the ESVDs by priority, since structures in Table I are generally arranged in descending order, read from left to right, by the Kekulé index provided below each structure.

In regards to claim 20, applicants argue that claim 20 defines systems for use in deriving fixed bond information and that Graovac et al. does not disclose or suggest these features. As recited for in a previous Office action, mailed 10/23/2003, Graovac et al. reasonably sets forth a system as recited in instant claim 20. Applicants arguments are found non-persuasive as the claimed system lack any specific limitations which would exclude such methodological systems as disclosed in the reference.

Conclusion

Any inquiry concerning this communication or earlier communications from the examiner should be directed to Eric S. DeJong whose telephone number is (571) 272-6099. The examiner can normally be reached on 8:30AM-5:00PM.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's supervisor, Ardin Marschel, Ph.D. can be reached on (571) 272-0718. The fax phone number for the organization where this application or proceeding is assigned is (571) 273-8300.

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Any inquiry of a general nature or relating to the status of this application should be directed to Legal Instrument Examiner, Tina Plunkett, whose telephone number is (571) 272-0549.

Information regarding the status of an application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information about the PAIR system, see <http://pair-direct.uspto.gov>. Should you have questions on access to the Private PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free).

Patent applicants with problems or questions regarding electronic images that can be viewed in the Patent Application Information Retrieval system (PAIR) can now contact the USPTO's Patent Electronic Business Center (Patent EBC) for assistance. Representatives are available to answer your questions daily from 6 am to midnight (EST). The toll free number is (866) 217-9197. When calling please have your application serial or patent number, the type of document you are having an image problem with, the number of pages and the specific nature of the problem. The Patent Electronic Business Center will notify applicants of the resolution of the problem within 5-7 business days. Applicants can also check PAIR to confirm that the problem has been corrected. The USPTO's Patent Electronic Business Center is a complete service center supporting all patent business on the Internet. The USPTO's PAIR system provides Internet-based access to patent application status and history information. It

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also enables applicants to view the scanned images of their own application file folder(s) as well as general patent information available to the public.

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John S. Brusca 8 Jun 2005
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PRIMARY EXAMINER